

09915515.072701

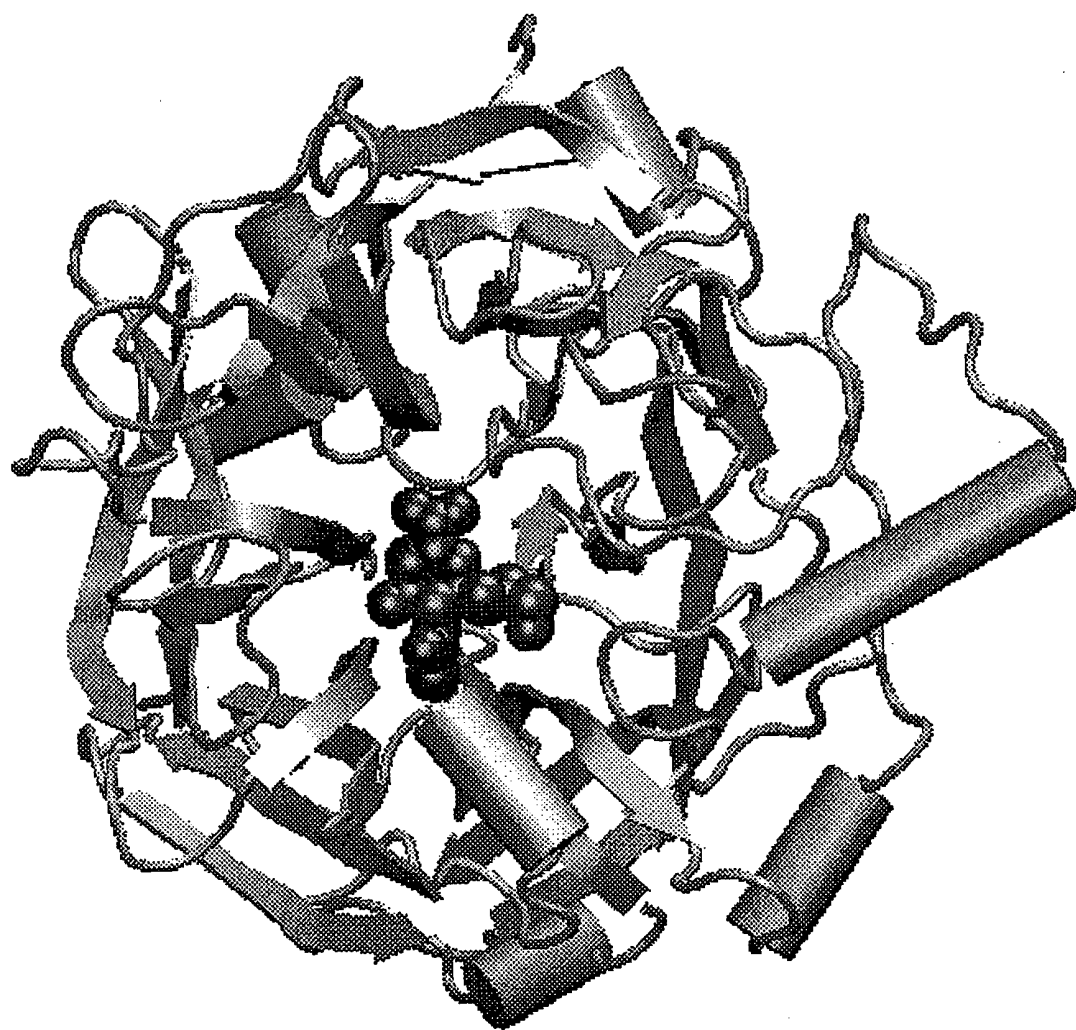


Fig. 1

09915515.072701

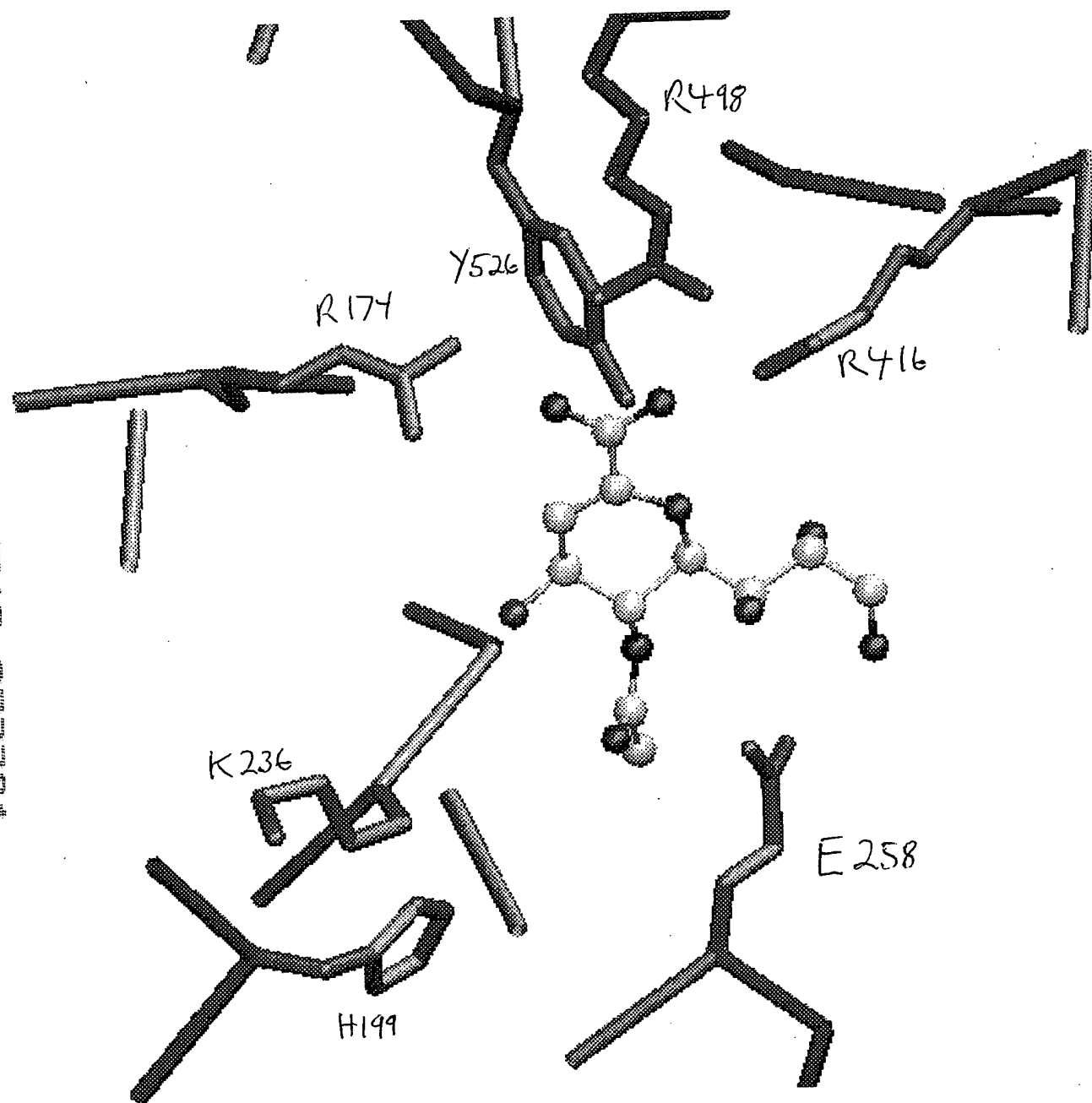


Fig. 3

09915515.072701

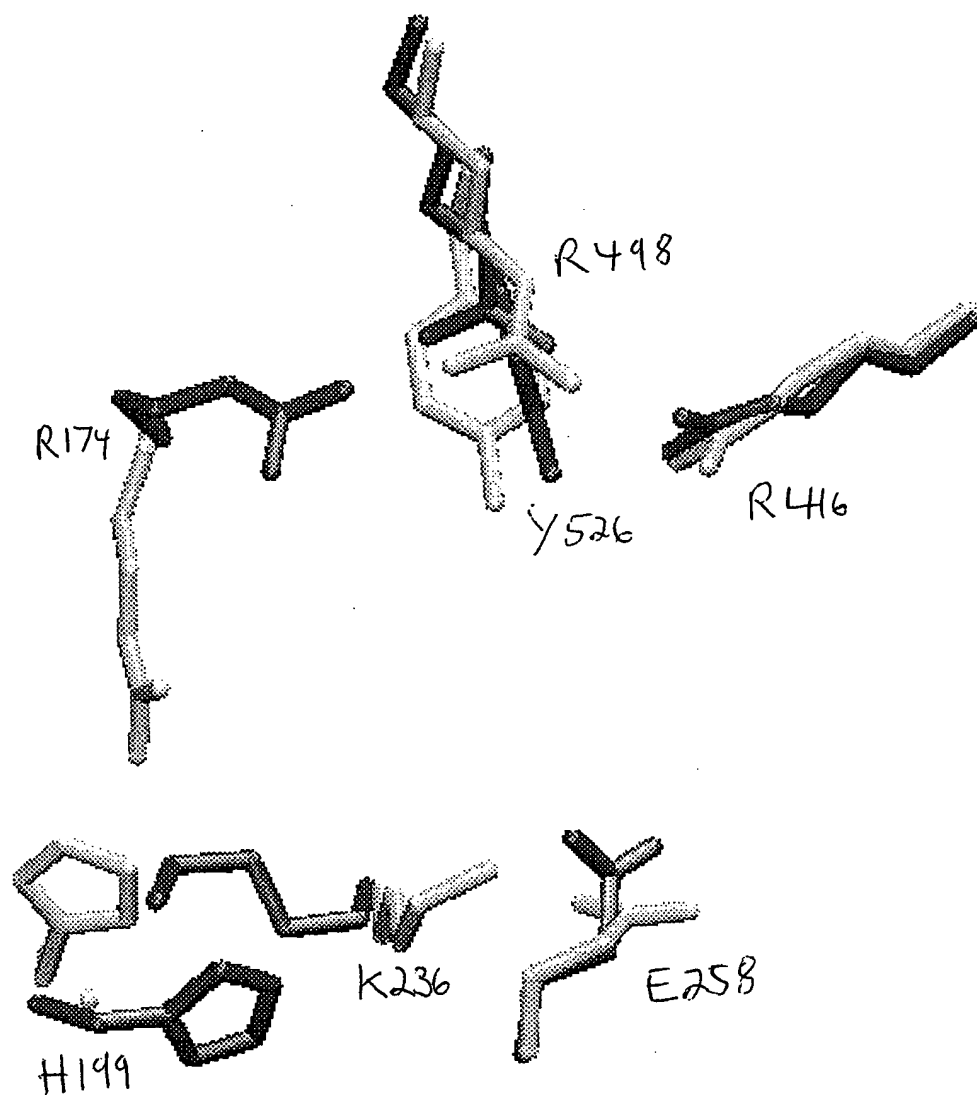


Fig. 4

09915515-072701

	Native 1	Native 2	Native 3	Native 4	NANA	DANA
Cell (Å)	73.3	72.3	71.7	72.0	71.6	137.5
	78.0	77.9	77.9	83.8	77.6	137.5
	202.6	199.2	198.2	201.5	197.2	116.6
Temp(K), pH	293, 7	100, 4.6	100, 4.6	293, 6	100K, 4.6	100K, 6.5
Resolution (Å)	3.0	2.0	2.5	3.0	2.5	2.8
# obs	172104	623166	420703	277932	210555	498619
# unique	20022	68217	38168	22207	29671	38673
Complete ness(%)	83	86	97	88	76	94
R _{merg} (%)	9.3	4.9	3.1	9.3	4.2	5.2
R-factor			0.222		.223	0.209
R _{free}			0.277		.291	0.235
# protein atoms			6914		6914	6896
# CHO, Ca,			89		116	111

Fig. 5

ligands

# waters	211	207	239
 A, B Å ²	25,36	32,44	44,44
 ligand Å ²		38,57	48,41

Table 1 Crystallographic data and refinement statistics.

Datasets Native2, Native3, NANA and DANA from frozen crystals were collected on beamlines X11 and BW7A at DESY, Hamburg. All other datasets were collected on in-house rotating anode and image plate or multiwire detector systems.

$R_{\text{merge}} = \sum_{hkl} \sum_i |\sum I_{hkl} - \langle I_{hkl} \rangle| / \sum_{hkl} \sum_i \langle I_{hkl} \rangle$ where the sum i is over all separate measurements of the unique reflections hkl .

$$R\text{-factor} = \sum_{hkl} ||F_{\text{obs}}| - |F_{\text{calc}}|| / \sum_{hkl} |F_{\text{obs}}|$$

R_{free} , as R-factor but summed over a 10% test set of reflections.